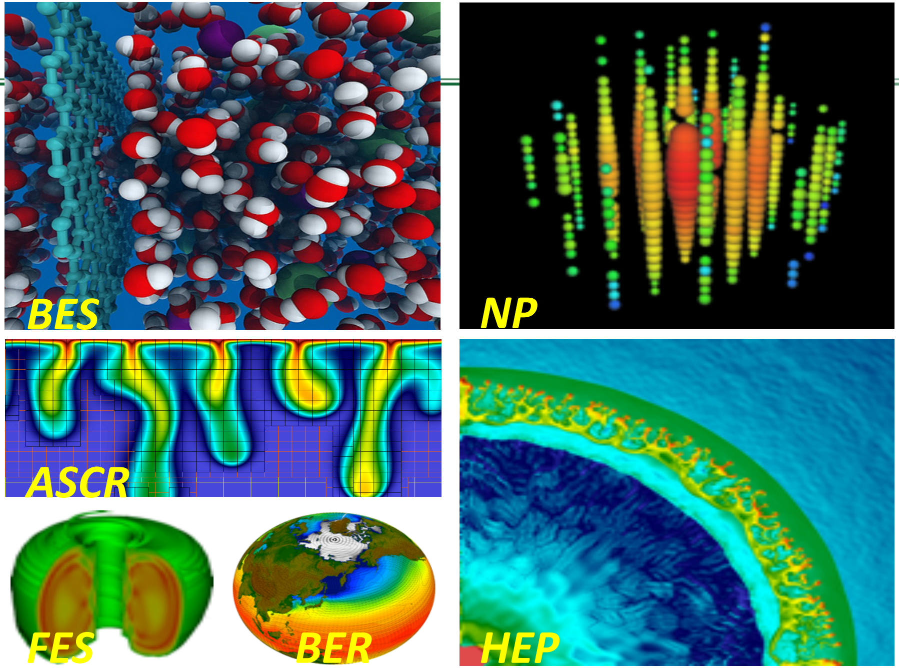
NERSC Science Highlights

June 2017



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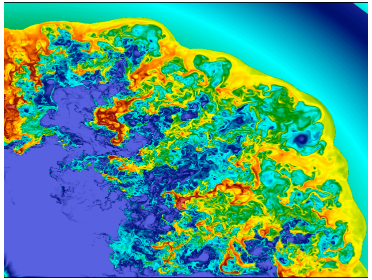
Science Highlights June 2017

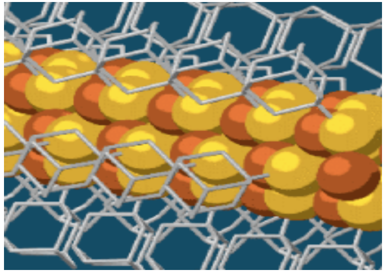
Astrophysics

First 2D models of rare superluminous supernova reveal insight into their origin.
NERSC PI: Woosley, UC Santa Cruz. ***Astrophysical Journal***



Materials Science

Researchers develop a process that promises to speed the discovery of commercially viable materials to produce solar fuels. **PI: Neaton, Berkeley Lab.** ***Proc. Nat. Acad. Sci.***



Materials Science

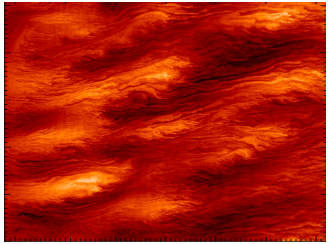
Scientists have discovered a way to use diamondoids to make electrical wires just 3 atoms wide. **NERSC PI: Devereaux, Stanford,** ***Nature Materials***

Atmospheric Science

3D models lead to an improved statistical representation of clouds. **NERSC PI: Ovchinnikov, Pacific NW Labs,** ***J. of Geophys. Rsrch: Atmospheres***

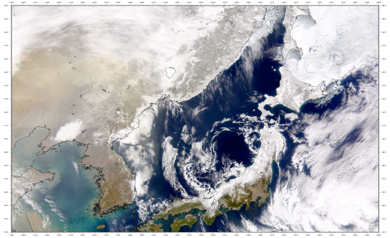
Fusion Energy

Researchers find multiscale electron energy transport in tokamak fusion reactors. **NERSC PI: Holland, UC San Diego.** ***Nuclear Fusion***



Environment

Simulations reveal that less dust leads to worse air pollution in China. **NERSC PI: Ghan, Pacific NW Labs.** ***Nature Communications***



Simulating Superluminous Supernova

Scientific Achievement

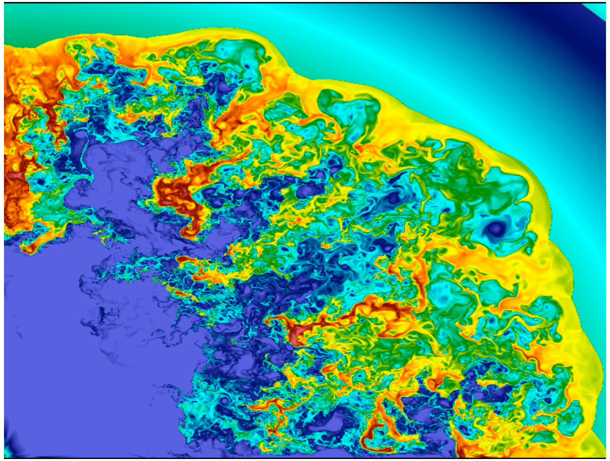
To better understand the processes that create rate and poorly understood superluminous supernova, astrophysicists completed the first two dimensional simulations of these rare events.

Significance and Impact

By modeling the exploding star in 2D, which is computationally intensive, researchers captured detailed information about fluid instabilities and mixing that isn't possible in 1D simulations. These details are important to accurately model the mechanisms that cause the event to be superluminous and explain their corresponding observational signatures, such as light curves and spectra.

Research Details.

Researchers from UC Santa Cruz used the CASTRO code , developed at Berkeley Lab, to run the simulations on NERSC's Edison supercomputer.



A 2D superluminous supernova simulation generated with the CASTRO code. (Image: Ken Chen, National Astronomical Observatory of Japan)

K. Chen, S. Woolsey, T. Sukhbold, The Astrophysical Journal, 832, 1, Nov. 2016

NERSC Project PI:
S. Woolsey, UC Santa Cruz

Turning Water into Fuel

Scientific Achievement

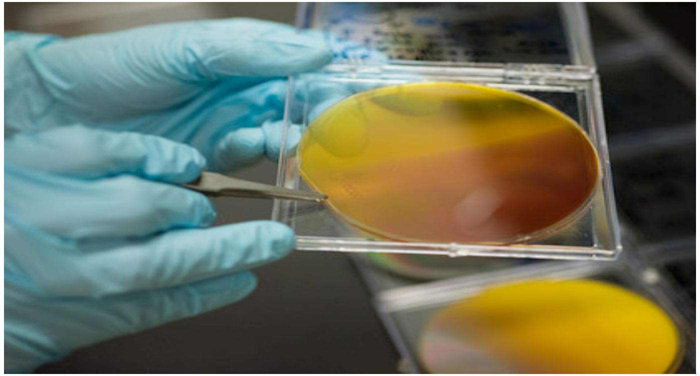
Solar fuels show promise as a clean-energy resource, but there are a limited number of materials with the necessary properties. Combining *ab initio* calculations run at NERSC with experiments, researchers from Caltech and Berkeley Lab developed a process that promises to speed the discovery of commercially viable materials.

Significance and Impact

Scientists have been trying to develop low-cost, efficient materials, known as photoanodes, that can act as a solar-powered catalyst to transform water into a hydrogen fuel. This research nearly doubled the number of materials known to have potential for use in solar fuels.

Research Details

- The researchers explored 174 metal vandates and identified 12 new potential photoanodes.
- The team learned more about the electronic structure of the materials.
- This study used data from the Materials Project hosted at NERSC.



Scientists at the the Joint Center for Artificial Photosynthesis at Caltech create new materials by spraying combinations of elements onto thin plates. Image credit: Caltech

Q. Yan et al, Proc. of the National Academy of Sciences, 114, 12, March 17, 2017

NERSC Project PI: J. Neaton, Berkeley Lab

World's Smallest Diamond Nanowires

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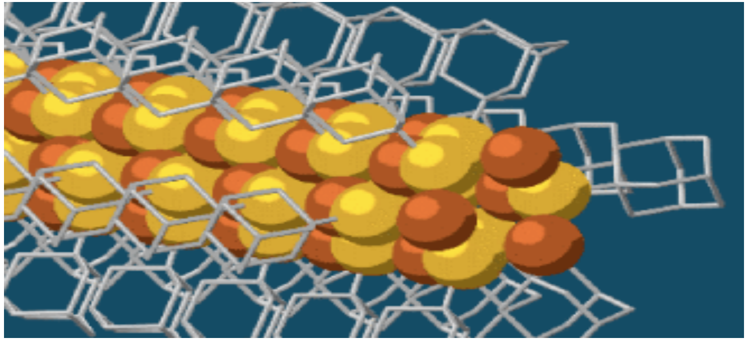
Scientific Achievement

Scientists at Stanford University and SLAC have discovered a way to use diamondoids – the smallest bits of diamond – to assemble atoms into the thinnest possible electrical wires, just 3 atoms wide.

Significance and Impact

By grabbing various types of atoms and putting them together LEGO-style, the new technique could potentially be used to build tiny wires for a wide range of applications, including fabrics that generate electricity, optoelectronic devices that employ both electricity and light, and superconducting materials that conduct electricity without any loss.



An illustration shows the basic nanowire building block – a diamondoid cage carrying atoms of copper and sulfur – drifting toward the growing tip of a nanowire, center, where it will attach in a way determined by its size and shape. Image credit: SLAC

Research Details

- Using supercomputers at NERSC, the research team modeled and predicted the electronic properties of the nanowires, which were examined with X-rays at SLAC's Stanford Synchrotron Radiation Light Source to determine their structure and other characteristics.

H. Yan, et al, Nature Materials, 16, 349-355, March 2017

NERSC Project PI:
T. Devereaux, Stanford

Cloud Modeling Goes Vertical

Scientific Achievement

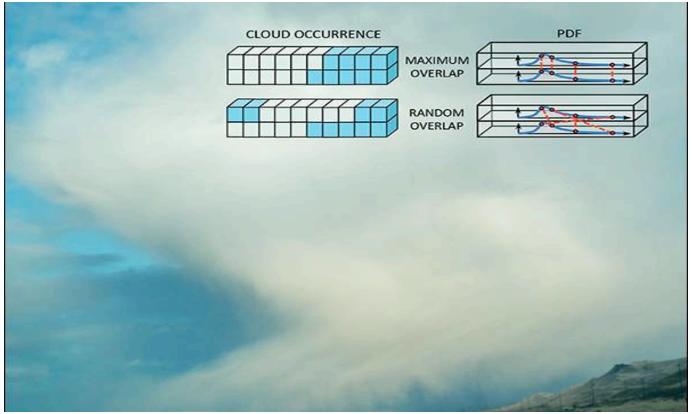
Researchers at Pacific Northwest National Laboratory improved a statistical representation of clouds that predicts how well cloud properties line up vertically and reveals how these vertical relationships depend on the type of cloud particles.

Significance and Impact

Clouds are difficult to represent in atmospheric models. They are constantly changing and vary in size, type, density, and other characteristics and currently can't be modeled directly in global models. Therefore accurate statistical treatments of vertical cloud distributions are vital in climate models.

Research Details

Using supercomputers at NERSC, the team ran detailed numerical simulations that explicitly represented the 3D structure of cloud and precipitation fields and analyzed these virtual clouds for statistical relationships between cloud and precipitation variables at different levels.



Streaks of precipitation show a higher vertical coherence, or near maximum line up, of fast-falling raindrops, while non-precipitating clouds have larger layer-to-layer variability—no streaks.
Image credit: Journal of Geophysical Research

M. Ovchinnikov, et al, J. of Geophysical Research: Atmospheres, 121, 21, Nov. 2016

NERSC Project PI: M. Ovchinnikov

Predicting Electron Energy Transport in ITER

Scientific Achievement

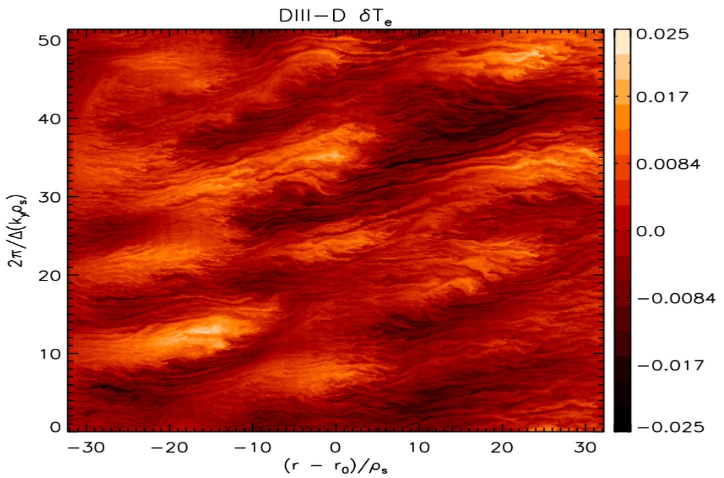
Multiscale fusion plasma simulations run at NERSC provide the first evidence that electron transport in tokamak plasmas such as those in ITER likely has a strong multiscale nature.

Significance and Impact

Accurately understanding electron transport in a fusion reactor is critical for predicting performance in future reactors like ITER. This study provides significant new evidence that electron energy transport in burning plasmas occurs over many scales and illustrates that simulations are vital for identifying phenomena in future reactors.

Research Details

- Through multiscale simulations run on Edison, researchers showed for the first time a complete suppression of long-wavelength turbulence.
- The researchers used between 3,072 cores for the smallest ion-scale simulations and 22,080 cores for the multiscale simulations.



Temperature fluctuations from a high-resolution simulation of a plasma discharge in the DIII-D tokamak. The DIII-D plasma was designed to match many of the parameters targeted for ITER. Image credit: Chris Holland, UCSD

C. Holland, N. Howard, B. Grierson, Nuclear Fusion 57, 2017, 066043

NERSC PI: C. Holland, UC San Diego

More Dust, Better Air Quality

NERSC

Scientific Achievement

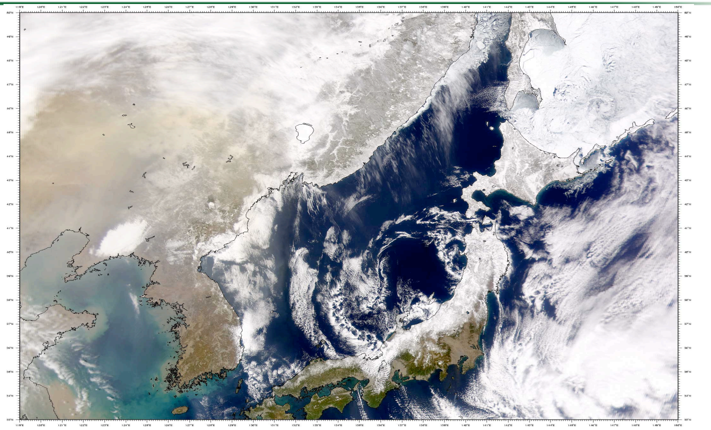
Man-made pollution in eastern China worsens when less dust blows in from the Gobi Desert, according to researchers from Pacific Northwest National Lab, Scripps Institution of Oceanography and UC San Diego.

Significance and Impact

Dust plays an important role in determining air temperatures and thereby promoting winds to blow away man-made pollution. Less dust means air stagnates, with pollution becoming more concentrated and sticking around longer.

Research Details

- Using computer models run at NERSC, together with historical data, the team found that reduced natural dust transported from the Gobi Desert translates to increased air pollution in highly populated eastern China.
- The results match observational data from dozen of sites in eastern China. The team found that two to three days after winds had brought dust into the region from western China, the air was cleaner than before the dust arrived.



Gobi Desert dust envelops eastern China. Image credit: SeaWiFS Project, NASA/Goddard Space Flight Center and ORBIMAGEE

Y. Yang, et al, Nature Communications 8, 15333, May 2017

NERSC Project PI: S. Ghan, PNNL

National Energy Research Scientific Computing Center